Clearing The Air: New Approaches to Life Support in Outer Space

# [DECK]

Jim Knox of the NASA Marshall Space Flight Center reports on research into atmospheric revitalization systems for long-term space travel and the use of COMSOL Multiphysics to understand how structured sorbents can be used to improve the performance of adsorption processes via thermal management.

#### [MAIN TEXT]

Beginning around the year 2020, NASA intends to return to the moon and to build a lunar outpost that will be staffed continuously by four astronauts on six-month shifts. Further in the future, the NASA vision for space exploration calls for a manned mission to Mars - a two to three-year roundtrip.

An engineering requisite for all space travel is the minimization of power, weight, and volume because all three translate to mass for any launch system. Compared to near-earth missions such as the International Space Station, manned lunar outposts and long-duration space travel present additional constraints that stress system engineering. Chief among these constraints is that every system must be robust enough to operate for long periods of time without compromising crew safety, without resupply, and without launch-taxing extra mass such as spare parts or a glut of backup equipment. Life support systems are no exception.

My colleagues and I at the Life Support Systems Development Team of NASA's Marshall Space Flight Center in Huntsville, Alabama, have been tasked with developing robust yet mass-minimizing life support systems for long-duration space travel, such as a roundtrip to Mars. Other integral members of our extended team are the adsorption experts at Vanderbilt University, led by M. Douglas LeVan, and at the University of South Carolina, led by James Ritter. Engineered structured sorbent (ESS) technologies and, in particular, sorbent-coated metal technologies appear to have the characteristics required to reduce both complexity and overall resource needs.

We are developing the next generation of atmosphere revitalization systems, which will reach for new levels of resource conservation via a high percentage of loop closure. For example, a high percentage of carbon dioxide, exhaled by crew, can be converted via reaction to drinking water, closing the loop from human metabolic waste to supply. Adsorption processes play a lead role in these new closed loop systems. However, loop closure requires additional energy and mass.

One new atmospheric revitalization technology we are investigating involves the coating of thermally and electrically conductive (generally metallic) substrates with molecular sieve sorbents. Molecular sieves provide a robust, safe, and stable adsorbent for the removal of metabolic CO<sub>2</sub> and water and reclamation for crew use. Use of a metallic substrate allows for direct and efficient sorbent heating as well as the capability to reduce the negative impacts of the heat of adsorption on process efficiency.

But sorbent-coated metal technologies present a number of tradeoffs in terms of working capacity, mass, and volume. Thus, the question becomes are they worth the effort? Multiphysics simulation plays a key role in our design and analysis process as we investigate that question.

### Current Life Support Technology

The average person produces about 1 kg of carbon dioxide and 2.33 kg of water as part of their normal daily metabolic process, with higher emission rates during strenuous physical activity. If you have ever entered a crowded room with insufficient air conditioning, you probably noted the stale air and high humidity. In the tightly sealed environment of a crew cabin, these conditions must be prevented since, at high concentrations, CO<sub>2</sub> can be poisonous and condensation forming on the electronics can wreak havoc on the systems vital to the mission.

The current life-support technology deployed in the International Space Station is a four-bed molecular sieve (4BMS). This system desiccates the process air prior to CO<sub>2</sub> removal and returns the captured water vapor back to the cabin air (see Figure 1). The system currently vents CO<sub>2</sub>, although with modifications it could store CO<sub>2</sub> in an accumulator for subsequent oxygen recovery. Highly effective, the 4BMS removes 100 percent of the metabolic CO<sub>2</sub> as well as some trace gases emitted by people and equipment.

The 4BMS system, however, has a number of drawbacks making it unsuitable for extended space forays. One of these shortcomings is due to the poor thermal conductivity of molecular sieves. As a result, indirect heating to assist desorption is inherently inefficient, requiring large amounts of power. The 4BMS also uses packed beds of pelletized sorbent materials, which tend to generate dust.

Problems such as these have led NASA to explore new designs for long-duration space travel. Solid sorbents such as zeolites coated on expanded metal or metal "foam" can be directly heated by sending an electrical current through the metallic substrate. This approach also provides a dust-free adsorption process for the removal of metabolic CO<sub>2</sub> and water.

### Conflicts with Heating and Cooling

In addition to solving the packed bed dusting problem, sorbent-coated metal ESS technologies also may offer the increased robustness and the reduced resource (power, weight, volume) requirements needed for the operation of a long-term life support systems. This becomes apparent considering the physics underlying adsorption and desorption processes. Heat, for example, is produced during adsorption yet the resulting higher temperatures reduce sorbent capacity and therefore inhibit adsorption. On the other hand, during desorption heat is lost and temperatures drop. While cooling increases sorbent capacity, it impedes desorption. The net effect of the heating and cooling byproduct of the adsorption process is a reduction in the working capacity of a regenerative revitalization system.

One potential solution to this problem lies in transferring the heat between adjacent adsorption and desorption beds to approach an isothermal process. This, along with the capability for direct resistive heating, led us to explore how Microlith<sup>TM</sup> substrates from Precision Combustion Incorporated and Electron Beam Melting (EBM) manufacturing substrates from Arcam behave when coated with zeolites.

Microlith<sup>TM</sup> is an expanded metal screen coated in a sorbent material (see Figure 2). When electrically heated, the intimate contact of Microlith<sup>TM</sup> metal and sorbent make for an efficient heat transport to the sorbent. But heat expands the metal and, due to the different coefficients of expansion, spalling of the coated sorbent can occur. Precision Combustion has developed a proprietary coating layering technology that has been shown to minimize spalling.

Simulations of a sorption canister (see Figure 3A) using Microlith<sup>TM</sup> separated by glass fibers to enable resistive heating indicate a uniform flow of gases (see Figure 3B). Further optimization of this design is needed, especially in regard to ways to reduce the volume of open area without causing flow maldistribution..

Arcam's EBM rapid manufacturing process uses an electron beam to melt metal powder that then fuses, layer by layer, into a part that might otherwise be impossible to machine (see Figure 4). Figure 4B shows a latticed part produced by this process, while Figure 4C shows a magnified section of an EBM lattice coated with sorbent.

With these technologies appearing hopeful, the next challenge facing us is, how to optimize the removal efficiency of a coated metal sorbent module, and thus reduce overall system volume? A second related question is, what sort of performance gains (and system size reductions) can be realized by removing the heat of adsorption during the carbon dioxide and humidity removal process? We address the second question first below.

#### Hot Beds of Sorbent

We built models of sorbent beds using COMSOL Multiphysics to learn more about the thermal characteristics of various sorbents under different physical phenomena. To derive the LDF (linear driver force) coefficient, we modeled isothermal adsorption testing conducted with a plate-finned heat exchanger packed with sorbent (ref. NASA CR 2277) (see Figure 5A).

Due to the relatively constant temperature within the canister, the heat of adsorption could be neglected allowing the mass transfer to be studied in isolation. Figure 5B shows the convection dispersion equations used to model the isothermal process. The LDF coefficient in the solid phase is  $k_{\rm ef}$ , q-bar is the actual amount absorbed, and  $q^*$  is the amount that would be absorbed at equilibrium. The difference between q-bar and  $q^*$  is the driving force for adsorption, analogous to temperature differences that provide the driving force for heat transfer.

Testing began with a completely clean sorbent bed and the introduction of CO<sub>2</sub> laden nitrogen (see Figure 5C). Initially, no CO<sub>2</sub> exits the bed, but then the CO<sub>2</sub> outlet history emerges in the classic S-curve shape of a breakthrough curve. By adjusting the k<sub>ef</sub> value, we obtained a match between the actual test data and the COMSOL simulation data.

We then looked at another test of water adsorption on silica gel with the same apparatus (see Figure 5D). After adjusting the  $k_{\rm ef}$  value for this process, data from the COMSOL Multiphysics simulation (red lines) once again provided a reasonable match with the actual inlet data (dotted lines).

Since these tests indicated we were on the right path, our next step was to characterize the thermal characteristics of a sorbent canister and to determine the heat transfer coefficient between the fluid and the sorbent and the fluid and the wall ( $h_s$  and  $h_w$  in Figure 6A). To do this, we called upon the apparatus shown in Figure 6B and 6C (ref. Mohamadinejad, H., Knox, J.C., and Smith, J. E. Experimental and Numerical Investigation of Adsorption/Desorption in Packed Sorption Beds under Ideal and Nonideal Flows. SEPARATION SCIENCE AND TECHNOLOGY, 2000, 35(1), 1-22.)

Here, we were looking at the heat balance for the gas phase. This testing started with a clean bed of sorbent material and introduced 350° Fahrenheit nitrogen, resulting in the large temperature swing shown in Figure 6D. Modeling results following adjustment of the heat-transfer coefficients (also shown in Figure 6D) provide in a good match between the test results and the COMSOL Multiphysics simulation. This gave us a usable characterization of the system.

After some additional testing and simulations, we were able to determine that eliminating the heat of adsorption would delay the initial breakthrough by about an hour, not an insignificant amount (see Figure 7). If we could adjust the actual adsorption cycle to take advantage of this delay, we could increase the adsorption performance and hence the working capacity. In a subscale test rig (Figure 8A), we proved that thermal recuperation using a granular silica gel with metallic foam could decrease the temperature changes in a sorption process by as much as 26° Fahrenheit depending upon the flow rate (see Figure 8B), and as a result, increase removal performance as much as 12% (see Figure 8C).

## Modeling the EBM Component

These results encouraged us to pursue our first question above, or how to optimize the removal efficiency of the coated metal sorbent, and thus reduce overall system volume? Optimization of the hardware and adsorption process requires understanding the effect of varying substrate geometry (metal strand size and spacing), process (flow, desorption method, and cycle time), and canister design (sorbent types and quantities). Multiphysics simulation was clearly required in order to capture effects of changing these parameters on the fluid dynamics, transient mass transfer, and transient heat transfer during the adsorption process.

Figure 9A shows an STL model of the interior lattice of the EBM part. Because meshing such a part would require enormous amounts of time and computing resources, we looked

first at an alternative interior design, which was simplified and easier to simulate (Figure 9B). The design features metal rods with a sorbent coating on their outside, with the rods connected thermally by a wall.

Still, even the alternate design was large to deal with, so we looked at a smaller subset of the design (Figure 10). The 2D image in Figure 10 is a 2D COMSOL Multiphysics simulation of a Navier-Stokes incompressible steady-state analysis of the flow field around the rods. The results we obtained from COMSOL showed us that the flow around the rods enters our adsorption chamber uniformly in the Y direction and quickly becomes an established, repeatable flow field.

With this data, we knew we could simplify our model further and zoom in on the physics and still obtain a reasonable answer. Next we examined the 3D flow, specifically the boundary layer effects on the flow away from the wall. Figure 11A shows the 3D COMSOL Multiphysics simulation of flow halfway across one of the beds of the structured sorbent lattice. Figure 11B shows the flow field in one of the eight boundary planes. Again, COMSOL Multiphysics indicates that the flow field becomes very consistent a short distance away from the wall (the x-axis). This meant that our next step is to optimize the rod size, spacing, and geometry to maximize the mass transfer from the fluid to the sorbent, while minimizing the pressure differential through the bed.

#### More to Come

So what does this all mean? For one, we know that the data generated thus far indicate that you can transfer the heat between adsorption and desorption beds in a sorbent-coated metal regenerative atmospheric revitalization system. A crucial milestone indicating that coated-metal ESS is worth the effort to learn more about.

But it also means that so much more work has to be done. For example, we have to develop more COMSOL Multiphysics simulations of existing subscale tests with EBM, Microliths, and other ESS sorbents. The process parameters (cycle time, flow rate, etc.) as well as the design and structure of the coated metal lattice work will also require a great deal more optimization through simulation. Then we have to build and test designs and compare alternate ESS approaches against packed bed sorbents, the present standard in the industry.

In short, we have many years of research prior to designing the TVSA atmospheric revitalization system for a trip to Mars and back. COMSOL Multiphysics has played a key role in our design and analysis process thus far, and our hope is to continue to use it extensively in the future.

#### About the Author

Jim Knox is the technical manager of the Sorbent-Based Atmosphere Revitalization project, developing CO<sub>2</sub> and H<sub>2</sub>O removal systems for the manned missions of NASA's Vision for Space Exploration. Mr. Knox has over 20 years experience from R&D work within the aerospace industry. Presently his focus is on the development of emerging

adsorption technologies for inclusion in future manned spacecraft carbon dioxide and humidity removal systems.

### [END MAIN TEXT]

# [CAPTIONS]

# FIGURE 1 = SLIDE 7 FROM KNOX COMSOL USER CONFERENCE PDF

Figure 1: The four-bed molecular sieve (4BMS) humidity and carbon removal system used in the International Space Station.

### FIGURE 2 = SLIDE 12 FROM KNOX COMSOL USER CONFERENCE PDF

Figure 2A: The Microlith expanded metal screen with a close-up

Figure 2B: Close-up of the Microlith expanded metal screen coated with sorbent.

Figure 2C: Precision Combustion's proprietary layering technology appears to have overcome problems with the sorbent spalling.

#### FIGURE 3 = SLIDE 13 FROM KNOX COMSOL USER CONFERENCE PDF

Figure 3A: An assembly showing the positioning of the Microlith expanded metal screen wrapped in glass fibers. The glass fibers enable electricity to be conducted through the metal to generate resistive heating that's key to the TVSA process.

Figure 3B: The simulation indicates the uniform flow of gases through and the need to reduce the flow volume.

# FIGURE 4 = SLIDE 14 FROM KNOX COMSOL USER CONFERENCE PDF

Figure 4a: An Arcam electronic beam rapid manufacturing machine made this part for the life support system in a single build by fusing powdered titanium.

Figure 4B: The interior lattice work of the part built by Arcam rapid manufacturing system.

Figure 4C: Close-up of an EBM sample coated with zeolite. An even tighter close up of the EBM sample coated with zeolite. The darker portions are the sorbent.

# FIGURE 5 = SLIDE 16 FROM KNOX COMSOL USER CONFERENCE PDF

Figure 5A: The heat exchanger model that was used for isothermal testing.

- Figure 5B: Convection dispersion equations used during isothermal testing.
- Figure 5C: Actual test data, represented by the dotted lines, shows that adjusting the K value matched the actual test data, which is represented by the dotted lines.
- Figure 5D: Water adsorption by silica gel. The actual outlet data are the dotted lines, while data generated by COMSOL Multiphysics are the solid red line.

#### FIGURE 6 = SLIDE 17 FROM KNOX COMSOL USER CONFERENCE PDF

- Figure 6A: The test apparatus used for determination of the heat transfer coefficient between the fluid and the sorbent and the fluid and the wall.
- Figure 6B: The equations used in the heat transfer simulation where h<sub>s</sub> and h<sub>w</sub> are the heat-transfer coefficient between the fluid and the sorbent and the fluid and the wall
- Figure 6C: A schematic representation of the test chamber, showing the locations of the sensing probes and the column of sorbent.
- Figure 6D: Test results and the COMSOL Multiphysics simulation provided a characterization of the heat phase.
- FIGURE 7 = SLIDE 19A FROM KNOX COMSOL USER CONFERENCE PDF
- Figure 7: Simulation of Theoretical Efficiency Improvement via Regenerative Heating.
- FIGURE 8 = SLIDE 23 FROM KNOX COMSOL USER CONFERENCE PDF Figure 8: Subscale VSA test results showing the performance improvement of thermally isolated sorbets beds as compared with a thermally linked bed.
- FIGURE 9 = SLIDE 25 FROM KNOX COMSOL USER CONFERENCE PDF
- Figure 9A: The actual STL file used to build the EBM lattice in Figure 4B.
- Figure 9B: An alternative and easier to model lattice showing metal rods coated in a sorbent and connected thermally by a wall in the middle.
- FIGURE 10 = SLIDE 26 FROM KNOX COMSOL USER CONFERENCE PDF
- Figure 10: This COMSOL Multiphysics image shows a uniformity of fluid flow through a 2D structured sorbent lattice in the Y direction.
- FIGURE 11 = SLIDE 27 FROM KNOX COMSOL USER CONFERENCE PDF
- Figure 11A: Fluid flow through structured sorbent lattice simulated in 3D by COMSOL Multiphysics.

Figure 11B: A close-up simulation of the flow fluid in COMSOL Multiphysics. The boundary layers are evident.

## [END CAPTIONS]

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## **ACKNOWLEDGMENTS**

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Figure 1

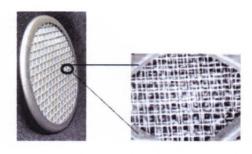


Figure 2A



Figure 2B

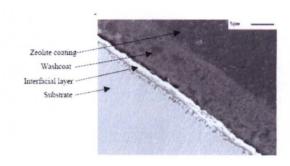


Figure 2C

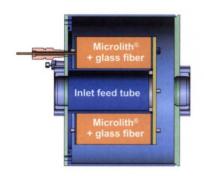


Figure 3A

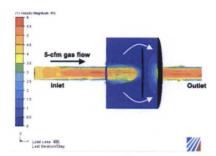


Figure 3B



Figure 4A

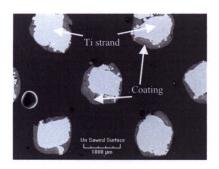


Figure 4C

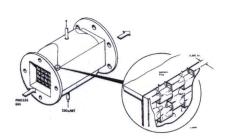


Figure 5A

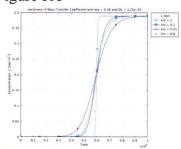


Figure 5C

Figure 4B

$$\begin{split} &\frac{\partial C_i}{\partial t} = D_1 \, \frac{\partial^2 C_i}{\partial x^2} - \frac{\partial u C_i}{\partial x} - \frac{1-\varepsilon}{\varepsilon} \, \frac{\partial \overline{q}_i}{\partial t} \\ &\text{at } t < 0, \, C_i = C_{i,0} \, \text{for } 0 \le x \le L \\ &\text{at } t < 0, \, \overline{q}_i = \overline{q}_{i,0} \, \text{for } 0 \le x \le L \\ &\text{at } t \ge 0, \, C_i = C_{i,0} \, \text{for } x = 0 \\ &\text{at } t \ge 0, \, \partial C_i / \partial x = 0 \, \text{for } x = L \\ &\partial \overline{q}_i / \partial t = k_{ef} a_e (q_i^* - \overline{q}_i) \end{split}$$

Figure 5B

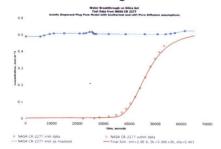


Figure 5D

$$\begin{split} \rho_{\mathrm{g}} c_{\mathrm{pg}} \, \frac{\partial T_{\mathrm{g}}}{\partial t} &= k_{f} \, \frac{\partial^{2} T_{\mathrm{g}}}{\partial x^{2}} - u \rho_{\mathrm{g}} c_{\mathrm{pg}} \, \frac{\partial T_{\mathrm{g}}}{\partial x} \\ &+ \frac{1 - \varepsilon}{\varepsilon} \, h_{\mathrm{s}} a_{\mathrm{s}} \, (T_{\mathrm{s}} - T_{\mathrm{g}}) - \frac{4 h_{\mathrm{w}}}{\varepsilon d} \, (T_{\mathrm{g}} - T_{\mathrm{w}}) \end{split}$$

Boundary and initial conditions:

at 
$$t < 0$$
,  $T_g = T_{g,0}$  for  $0 \le x \le L$   
at  $t \ge 0$ ,  $T_g = T_i$  for  $x = 0$   
at  $t \ge 0$ ,  $\partial T_g/\partial x = 0$  for  $x = L$ 

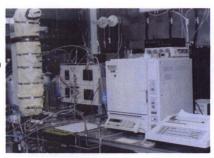


Figure 6B

Figure 6A

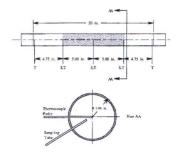


Figure 6C

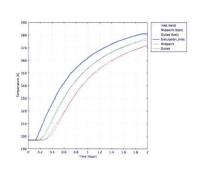


Figure 6D

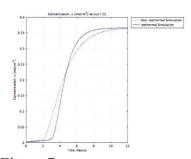


Figure 7



Figure 8A

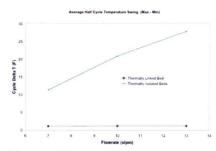


Figure 8B

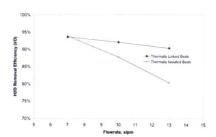


Figure 8C

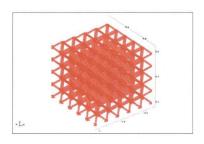


Figure 9A

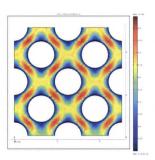


Figure 10

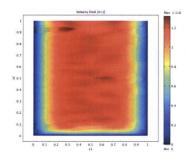


Figure 11B

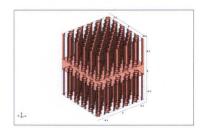


Figure 9B

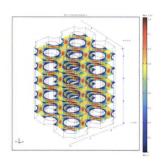


Figure 11A